Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:19 AM GMT

PDB ID	:	3E6O
Title	:	Structure of murine INOS oxygenase domain with inhibitor AR-C124355
Authors	:	Garcin, E.D.; Arvai, A.S.; Rosenfeld, R.J.; Kroeger, M.D.; Crane, B.R.; Andersson, G.; Andrews, G.; Hamley, P.J.; Mallinder, P.R.; Nicholls, D.J.; St-Gallay, S.A.; Tinker, A.C.; Gensmantel, N.P.; Mete, A.; Cheshire, D.R.; Connolly, S.; Stueh, D.J.; Aberg, A.; Wallace, A.V.; Tainer, J.A.; Getzoff, E.D.
Deposited on	:	2008-08-15
Resolution	:	2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

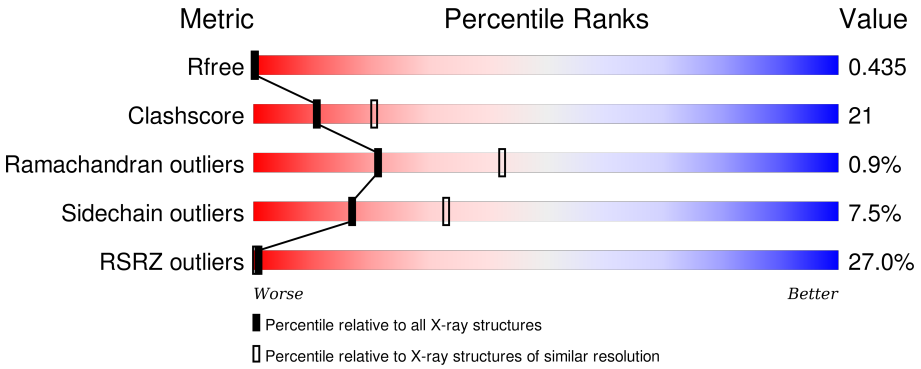
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	433	24% 56% 37%
1	B	433	28% 60% 30% 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	H4B	A	902	X	-	-	-
4	A55	B	904	-	-	-	X

2 Entry composition

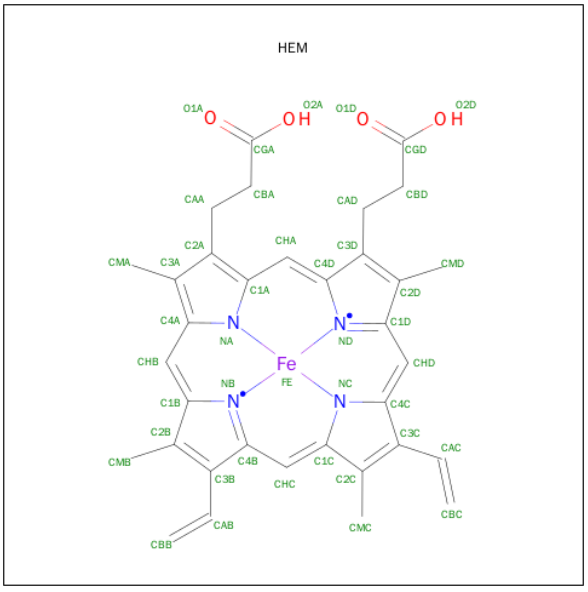
There are 5 unique types of molecules in this entry. The entry contains 7171 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Nitric oxide synthase, inducible.

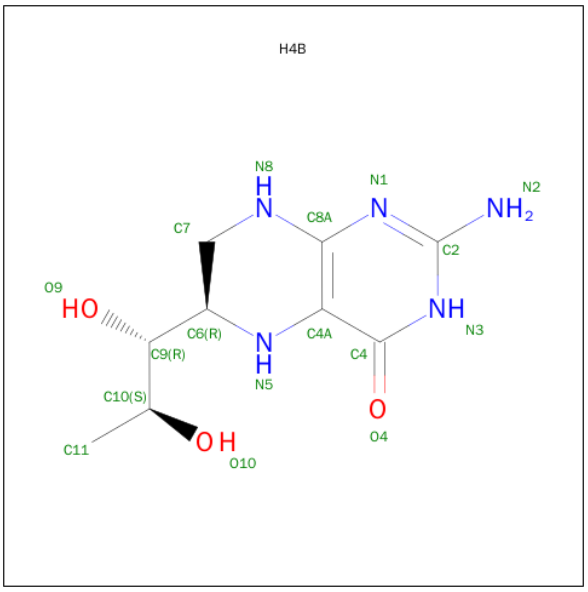
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	415	Total	C	N	O	S	0	0	0
			3385	2171	582	612	20			
1	B	410	Total	C	N	O	S	0	0	0
			3347	2148	577	602	20			

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



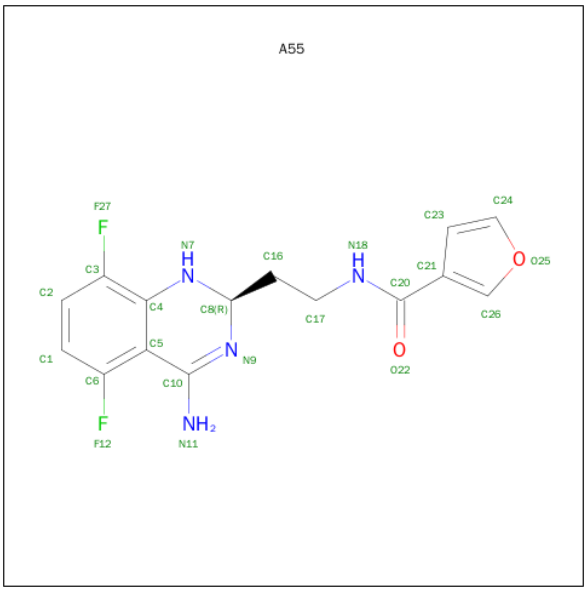
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is 5,6,7,8-TETRAHYDROBIOPTERIN (three-letter code: H4B) (formula: $C_9H_{15}N_5O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 17 9 5 3	0	0
3	B	1	Total C N O 17 9 5 3	0	0

- Molecule 4 is N-[2-(4-AMINO-5,8-DIFLUORO-1,2-DIHYDROQUINAZOLIN-2-YL)ETHYL]-3-FURAMIDE (three-letter code: A55) (formula: $C_{15}H_{14}F_2N_4O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C F N O 23 15 2 4 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	F	N	O	0	0
			23	15	2	4	2		

- Molecule 5 is water.

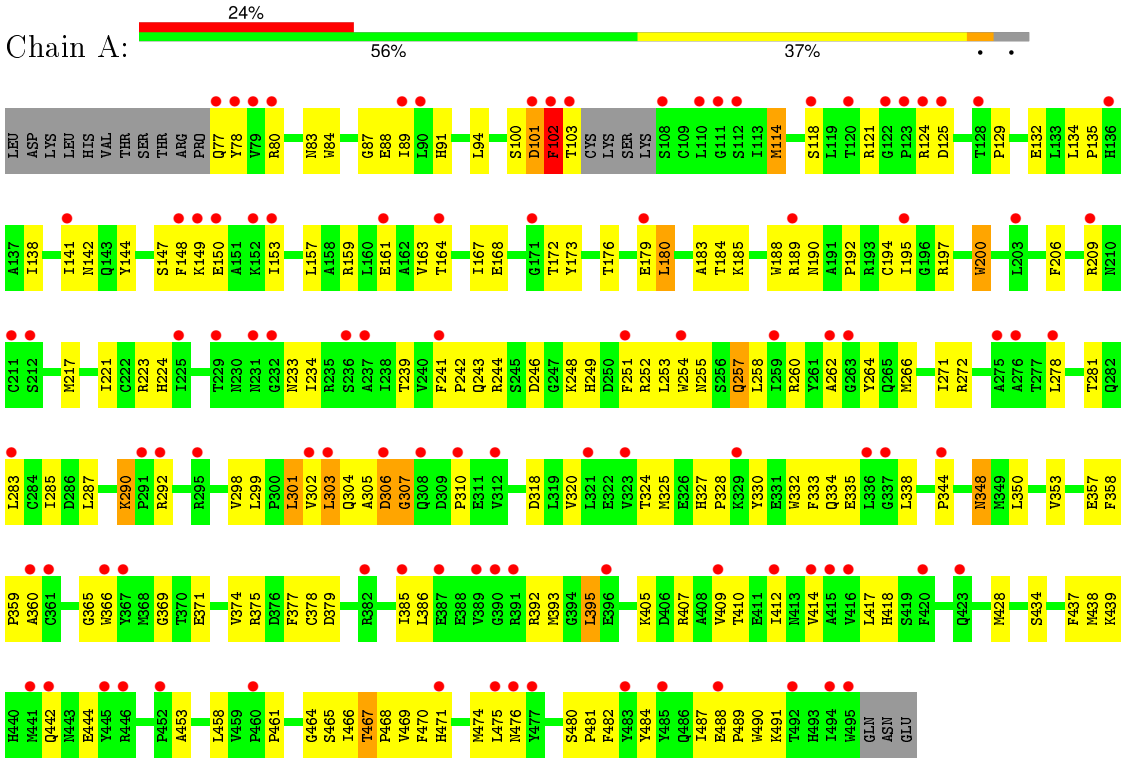
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	120	Total	O	0	0
			120	120		
5	B	153	Total	O	0	0
			153	153		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

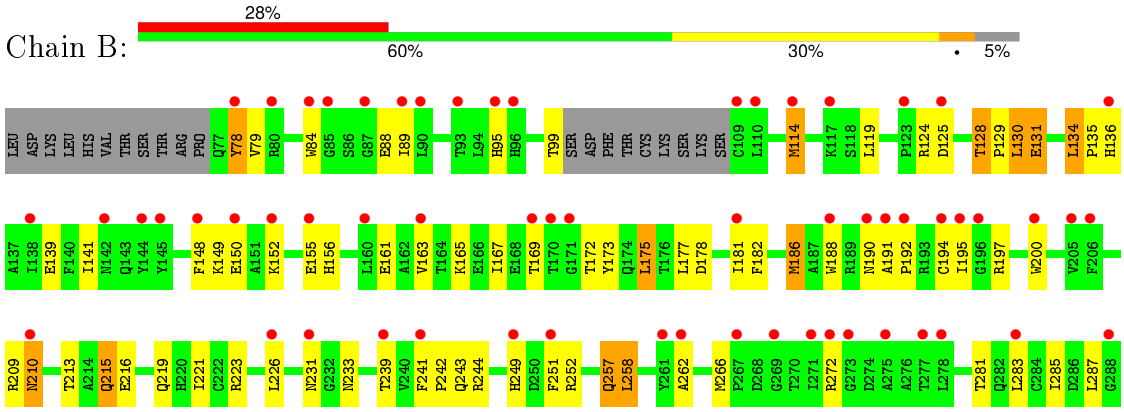
- Molecule 1: Nitric oxide synthase, inducible

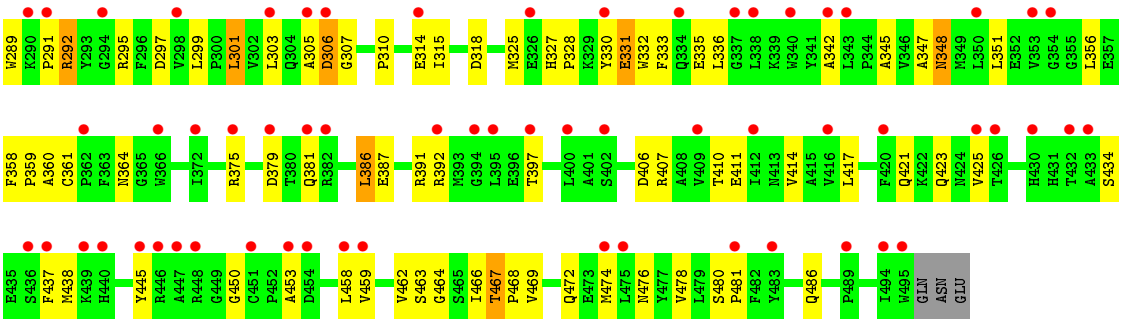
Chain A:



- Molecule 1: Nitric oxide synthase, inducible

Chain B:




W289 K290 P291 R292 Y293 G294 R295 F296 D297 V298 L299 P300 L301 V302 L303 Q304 A305 D306 G307 P310 E314 I315 D318 M325 E326 H327 P328 K329 Y330 E331 W332 F333 Q334 E335 L336 G337 L338 K339 W340 Y341 A342 L343 P344 A345 V346 A347 N348 W349 L350 L351 E352 V353 G354 G355 L356 E357
F358 P359 A360 C361 P362 F363 N364 G365 W366 I372 R375 D379 T380 Q381 R382 L386 E387 R391 R392 M393 G394 L395 E396 T397 L400 A401 S402 D406 R407 A408 V409 T410 E411 I412 N413 V414 A415 V416 L417 F420 Q421 K422 Q423 N424 V425 T426 H430 H431 T432 A433 S434
E435 S436 F437 M438 K439 H440 Y445 R446 A447 R448 G449 G450 C451 P452 A453 D454 L458 V459 V462 S463 G464 S465 I466 T467 P468 V469 Q472 E473 M474 L475 N476 Y477 V478 L479 S480 P481 F482 Y483 Q486 P489 I494 W495 GLN ASN GLU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α, β, γ	213.90Å 213.90Å 116.15Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.96 – 2.60 19.95 – 2.51	Depositor EDS
% Data completeness (in resolution range)	99.3 (19.96-2.60) 92.4 (19.95-2.51)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.49 (at 2.50Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.229 , 0.262 0.419 , 0.435	Depositor DCC
R_{free} test set	2049 reflections (4.14%)	DCC
Wilson B-factor (Å^2)	42.1	Xtriage
Anisotropy	0.786	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 56.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 53193 reflections	Xtriage
F_o,F_c correlation	0.74	EDS
Total number of atoms	7171	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.12% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, A55, H4B

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.40	0/3484	0.63	1/4737 (0.0%)
1	B	0.37	0/3445	0.62	0/4684
All	All	0.38	0/6929	0.63	1/9421 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	365	GLY	N-CA-C	-5.94	98.25	113.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3385	0	3278	158	4
1	B	3347	0	3248	125	4
2	A	43	0	30	3	0
2	B	43	0	30	1	0
3	A	17	0	14	0	1
3	B	17	0	14	0	0
4	A	23	0	14	0	0
4	B	23	0	14	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	120	0	0	12	1
5	B	153	0	0	10	1
All	All	7171	0	6642	285	8

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 21.

All (285) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:195:ILE:HB	5:B:1937:HOH:O	1.33	1.26
1:A:195:ILE:HB	5:A:1043:HOH:O	1.43	1.18
1:A:153:ILE:HD12	1:A:153:ILE:H	1.31	0.94
1:A:428:MET:HB3	5:A:1050:HOH:O	1.74	0.87
1:A:188:TRP:CE3	1:A:200:TRP:HA	2.15	0.81
1:A:141:ILE:HD11	1:A:163:VAL:HG21	1.65	0.79
1:B:292:ARG:HH11	1:B:292:ARG:HB2	1.48	0.79
1:A:195:ILE:HG12	1:A:458:LEU:HD22	1.64	0.79
1:B:129:PRO:HB2	1:B:131:GLU:OE2	1.85	0.75
1:A:102:PHE:C	1:A:103:THR:HG23	2.06	0.74
1:B:221:ILE:HG21	1:B:301:LEU:HD21	1.67	0.74
1:A:217:MET:CE	1:A:303:LEU:HB3	2.18	0.73
1:A:290:LYS:CE	1:A:290:LYS:H	2.03	0.72
1:B:215:GLN:HG2	5:B:1949:HOH:O	1.89	0.71
1:A:189:ARG:HD2	1:A:200:TRP:CE3	2.26	0.71
1:A:281:THR:O	1:A:285:ILE:HG12	1.90	0.71
1:A:407:ARG:HG3	1:A:407:ARG:HH11	1.56	0.70
1:B:197:ARG:NE	5:B:2015:HOH:O	2.23	0.70
1:A:304:GLN:O	1:A:304:GLN:HG3	1.91	0.70
1:B:215:GLN:O	1:B:219:GLN:HG3	1.92	0.70
1:B:467:THR:CG2	1:B:469:VAL:HG22	2.22	0.68
1:A:102:PHE:O	1:A:102:PHE:CG	2.45	0.68
1:B:301:LEU:HD13	1:B:315:ILE:HD11	1.75	0.68
1:A:290:LYS:CD	1:A:290:LYS:H	2.08	0.67
1:A:102:PHE:O	1:A:103:THR:HG23	1.95	0.67
1:B:195:ILE:CG2	1:B:437:PHE:HB2	2.25	0.67
1:A:188:TRP:CZ3	1:A:200:TRP:HA	2.30	0.67
1:B:188:TRP:CE3	1:B:200:TRP:HA	2.30	0.66
1:A:195:ILE:HD11	1:A:458:LEU:O	1.95	0.66
1:A:141:ILE:CD1	1:A:163:VAL:HG21	2.24	0.66
1:A:333:PHE:HB3	5:A:1099:HOH:O	1.95	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:210:ASN:N	1:B:210:ASN:HD22	1.94	0.66
1:B:197:ARG:CZ	5:B:2015:HOH:O	2.43	0.65
1:A:252:ARG:HD3	1:A:359:PRO:HB2	1.77	0.65
1:B:190:ASN:O	1:B:192:PRO:HD3	1.97	0.65
1:B:464:GLY:O	1:B:467:THR:HB	1.96	0.64
1:A:465:SER:O	1:A:471:HIS:HE1	1.80	0.64
1:B:149:LYS:HG2	1:B:150:GLU:HG3	1.78	0.64
1:B:141:ILE:HD11	1:B:163:VAL:HG21	1.79	0.64
1:B:210:ASN:H	1:B:210:ASN:HD22	1.43	0.64
1:A:144:TYR:O	1:A:147:SER:HB3	1.97	0.64
1:B:244:ARG:HA	5:B:1958:HOH:O	1.96	0.64
1:A:217:MET:HE1	1:A:303:LEU:HB3	1.80	0.64
1:A:195:ILE:HG22	1:A:195:ILE:O	1.98	0.63
1:A:217:MET:HE2	1:A:305:ALA:HB2	1.81	0.62
1:B:195:ILE:HD11	1:B:458:LEU:O	2.00	0.62
1:A:217:MET:HE3	1:A:303:LEU:HB3	1.81	0.62
1:A:410:THR:O	1:A:414:VAL:HG23	2.00	0.62
1:B:467:THR:HG21	1:B:469:VAL:HG22	1.81	0.61
1:A:124:ARG:HD3	5:A:1020:HOH:O	1.99	0.61
1:A:290:LYS:HE3	1:A:290:LYS:H	1.65	0.61
1:B:292:ARG:NH1	1:B:297:ASP:HB3	2.16	0.61
1:A:334:GLN:HA	5:A:1098:HOH:O	2.00	0.61
1:B:209:ARG:O	1:B:242:PRO:HG3	2.00	0.61
1:A:224:HIS:ND1	1:A:239:THR:HG23	2.16	0.61
1:A:206:PHE:HB2	1:A:239:THR:HG22	1.83	0.61
1:B:249:HIS:C	1:B:306:ASP:O	2.39	0.60
1:A:84:TRP:NE1	1:A:114:MET:HG3	2.15	0.60
1:B:387:GLU:HG3	1:B:397:THR:HG21	1.84	0.60
1:B:195:ILE:HG22	1:B:195:ILE:O	2.02	0.60
1:A:221:ILE:HG21	1:A:301:LEU:HD21	1.84	0.60
1:A:332:TRP:CE3	1:A:392:ARG:HD2	2.37	0.59
1:B:285:ILE:HD11	1:B:291:PRO:HB3	1.84	0.59
1:B:210:ASN:H	1:B:210:ASN:ND2	1.99	0.59
1:A:246:ASP:OD2	1:A:248:LYS:HB3	2.02	0.59
1:B:177:LEU:O	1:B:181:ILE:HD13	2.03	0.59
1:B:301:LEU:HG	1:B:303:LEU:HD11	1.83	0.59
1:B:445:TYR:CE2	1:B:450:GLY:HA2	2.37	0.59
1:A:134:LEU:O	1:A:138:ILE:HG12	2.02	0.59
1:B:141:ILE:CD1	1:B:163:VAL:HG21	2.32	0.59
1:A:252:ARG:HB2	1:A:304:GLN:HG2	1.83	0.59
1:A:149:LYS:HG2	1:A:150:GLU:HG2	1.85	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:THR:OG1	1:B:216:GLU:HG3	2.03	0.58
1:B:438:MET:HG3	1:B:468:PRO:HB2	1.86	0.58
1:A:290:LYS:H	1:A:290:LYS:HD2	1.68	0.58
1:B:149:LYS:HG2	1:B:150:GLU:N	2.19	0.58
1:B:281:THR:O	1:B:285:ILE:HG12	2.04	0.58
1:A:249:HIS:C	1:A:306:ASP:O	2.42	0.57
1:B:130:LEU:CD2	1:B:167:ILE:HG22	2.34	0.57
1:A:149:LYS:HG2	1:A:150:GLU:N	2.19	0.57
1:A:407:ARG:HG3	1:A:407:ARG:NH1	2.20	0.56
1:A:223:ARG:HD3	5:A:1061:HOH:O	2.04	0.56
1:B:195:ILE:HG23	1:B:437:PHE:HB2	1.87	0.56
1:A:132:GLU:O	1:A:135:PRO:HD2	2.06	0.56
1:B:84:TRP:CD1	1:B:114:MET:HE2	2.41	0.56
1:B:195:ILE:HG22	1:B:437:PHE:HB2	1.87	0.56
1:B:410:THR:O	1:B:414:VAL:HG13	2.06	0.56
1:B:156:HIS:ND1	5:B:1922:HOH:O	2.33	0.56
1:B:130:LEU:HD21	1:B:167:ILE:HG22	1.87	0.55
1:B:221:ILE:HD12	1:B:303:LEU:HD21	1.88	0.55
1:B:459:VAL:HG22	1:B:469:VAL:HG23	1.88	0.55
1:B:292:ARG:HH11	1:B:292:ARG:CB	2.18	0.55
1:A:439:LYS:O	1:A:442:GLN:HG2	2.07	0.54
1:B:152:LYS:HD2	1:B:155:GLU:OE2	2.07	0.54
1:B:445:TYR:HA	1:B:450:GLY:H	1.73	0.54
1:B:239:THR:O	1:B:361:CYS:HA	2.07	0.54
1:A:209:ARG:O	1:A:242:PRO:HG3	2.07	0.54
1:A:283:LEU:O	1:A:287:LEU:HG	2.07	0.54
1:A:405:LYS:O	1:A:409:VAL:HG23	2.08	0.54
1:A:176:THR:OG1	1:A:179:GLU:HG3	2.08	0.54
1:A:129:PRO:HB2	1:A:132:GLU:HG3	1.90	0.53
1:B:175:LEU:HD13	1:B:356:LEU:CD1	2.37	0.53
1:A:189:ARG:HD2	1:A:200:TRP:CZ3	2.42	0.53
1:A:290:LYS:HD3	1:A:292:ARG:HH22	1.74	0.53
1:A:438:MET:HG3	1:A:468:PRO:HB2	1.90	0.53
1:A:332:TRP:O	1:A:335:GLU:HB2	2.08	0.53
1:B:195:ILE:HG12	1:B:458:LEU:HD22	1.91	0.53
1:B:191:ALA:O	1:B:197:ARG:NH1	2.42	0.53
1:A:195:ILE:CG2	1:A:437:PHE:HB2	2.38	0.52
1:B:330:TYR:HB3	1:B:332:TRP:CE2	2.44	0.52
1:B:131:GLU:CD	1:B:131:GLU:H	2.13	0.52
1:A:303:LEU:O	1:A:310:PRO:HA	2.09	0.52
1:B:331:GLU:HA	1:B:331:GLU:OE1	2.08	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:PHE:HD2	1:A:239:THR:HG22	1.74	0.52
1:B:387:GLU:O	1:B:391:ARG:HG3	2.09	0.52
1:A:257:GLN:OE1	1:A:260:ARG:NH1	2.36	0.52
1:B:194:CYS:O	1:B:197:ARG:HG3	2.10	0.52
1:A:264:TYR:HB2	1:A:266:MET:CE	2.40	0.52
1:B:332:TRP:O	1:B:335:GLU:HB2	2.09	0.52
1:A:480:SER:HA	1:A:481:PRO:C	2.29	0.52
1:A:262:ALA:HB2	1:A:299:LEU:CD2	2.40	0.52
1:A:172:THR:OG1	1:A:173:TYR:N	2.42	0.51
1:A:185:LYS:O	1:A:189:ARG:HG3	2.09	0.51
1:B:438:MET:CE	1:B:469:VAL:HG12	2.41	0.51
1:B:177:LEU:HD13	1:B:181:ILE:HD13	1.91	0.51
1:B:78:TYR:CD1	1:B:78:TYR:C	2.84	0.51
1:B:333:PHE:HA	1:B:336:LEU:CD2	2.40	0.51
1:B:243:GLN:HB3	1:B:358:PHE:CE2	2.45	0.51
1:A:159:ARG:O	1:A:163:VAL:HG23	2.10	0.51
1:A:434:SER:HB3	1:A:468:PRO:HD2	1.91	0.51
1:A:453:ALA:HB3	1:A:474:MET:HB3	1.91	0.51
1:A:301:LEU:HB3	1:A:303:LEU:HD13	1.91	0.51
1:A:290:LYS:N	1:A:290:LYS:HE3	2.25	0.51
1:A:438:MET:HE2	1:A:469:VAL:HG12	1.94	0.50
1:A:464:GLY:O	1:A:467:THR:HB	2.12	0.50
1:A:164:THR:O	1:A:168:GLU:HG2	2.12	0.50
1:A:241:PHE:HB3	1:A:242:PRO:CD	2.40	0.50
1:B:124:ARG:HH21	1:B:128:THR:HB	1.76	0.50
1:B:327:HIS:ND1	1:B:328:PRO:HD2	2.26	0.50
1:A:190:ASN:O	1:A:192:PRO:HD3	2.12	0.50
1:A:153:ILE:HD12	1:A:153:ILE:N	2.14	0.50
1:B:165:LYS:O	1:B:169:THR:HG23	2.12	0.50
1:B:434:SER:HB3	1:B:468:PRO:HD2	1.94	0.50
1:A:138:ILE:HG22	1:A:142:ASN:HD21	1.76	0.50
1:B:251:PHE:O	1:B:360:ALA:HB2	2.11	0.50
1:A:195:ILE:HG23	1:A:437:PHE:HB2	1.94	0.50
1:B:188:TRP:CZ3	1:B:200:TRP:HA	2.47	0.50
1:A:327:HIS:ND1	1:A:328:PRO:HD2	2.27	0.50
1:A:241:PHE:HB3	1:A:242:PRO:HD2	1.94	0.49
1:A:233:ASN:ND2	5:A:1066:HOH:O	2.44	0.49
1:A:438:MET:CE	1:A:469:VAL:HG12	2.42	0.49
1:A:298:VAL:HG21	1:A:320:VAL:HG11	1.93	0.49
1:B:411:GLU:O	1:B:414:VAL:HG22	2.13	0.49
1:B:379:ASP:HB3	1:B:381:GLN:OE1	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:ILE:HG22	1:A:142:ASN:ND2	2.28	0.49
1:B:195:ILE:HG23	1:B:437:PHE:CB	2.43	0.49
1:A:467:THR:HG21	1:A:469:VAL:HG22	1.95	0.49
1:A:129:PRO:HG3	5:A:1021:HOH:O	2.13	0.48
1:B:445:TYR:CZ	1:B:450:GLY:HA2	2.48	0.48
1:A:88:GLU:HG2	1:A:89:ILE:N	2.28	0.48
1:A:290:LYS:HG2	1:A:292:ARG:HH12	1.77	0.48
1:B:131:GLU:CD	1:B:131:GLU:N	2.67	0.48
1:B:330:TYR:HB3	1:B:332:TRP:NE1	2.29	0.48
1:A:467:THR:CG2	1:A:469:VAL:HG22	2.44	0.48
1:A:244:ARG:HD2	1:A:357:GLU:OE2	2.13	0.48
1:B:295:ARG:HD2	5:B:2027:HOH:O	2.14	0.48
1:A:78:TYR:CD1	1:A:78:TYR:C	2.87	0.48
1:B:285:ILE:CD1	1:B:291:PRO:HB3	2.44	0.47
1:B:252:ARG:HD3	1:B:359:PRO:HB2	1.96	0.47
1:A:132:GLU:C	1:A:135:PRO:HD2	2.35	0.47
1:B:303:LEU:O	1:B:310:PRO:HA	2.15	0.47
1:A:330:TYR:HD2	1:A:332:TRP:HE1	1.62	0.47
1:A:252:ARG:CD	1:A:359:PRO:HB2	2.44	0.47
1:A:180:LEU:O	1:A:184:THR:HG23	2.14	0.47
1:A:301:LEU:HB3	1:A:303:LEU:CD1	2.45	0.47
1:B:241:PHE:HB3	1:B:242:PRO:CD	2.44	0.47
1:A:348:ASN:ND2	1:A:348:ASN:H	2.13	0.47
1:A:487:ILE:N	1:A:487:ILE:HD12	2.30	0.47
1:A:102:PHE:C	1:A:103:THR:O	2.53	0.47
1:B:438:MET:HE2	1:B:469:VAL:HG12	1.97	0.47
1:A:360:ALA:HA	5:A:1075:HOH:O	2.14	0.47
2:A:901:HEM:HMC1	2:A:901:HEM:HBC2	1.97	0.47
1:A:103:THR:O	1:A:103:THR:OG1	2.31	0.46
1:A:80:ARG:NH1	5:A:1136:HOH:O	2.48	0.46
1:A:78:TYR:CE1	1:A:91:HIS:ND1	2.82	0.46
1:A:189:ARG:HH21	1:A:444:GLU:CD	2.19	0.46
1:A:243:GLN:HB3	1:A:358:PHE:CE2	2.50	0.46
1:B:292:ARG:HD3	1:B:292:ARG:N	2.30	0.46
1:A:393:MET:HB2	1:A:395:LEU:HD22	1.96	0.46
1:A:305:ALA:O	1:A:307:GLY:N	2.49	0.46
1:B:194:CYS:O	1:B:197:ARG:NH1	2.49	0.46
1:A:290:LYS:CD	1:A:290:LYS:N	2.77	0.46
1:A:253:LEU:HD12	1:A:253:LEU:N	2.30	0.46
1:A:290:LYS:N	1:A:290:LYS:HD2	2.30	0.46
1:B:241:PHE:HB3	1:B:242:PRO:HD2	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:THR:N	1:B:216:GLU:OE1	2.50	0.45
1:A:271:ILE:HD13	1:A:278:LEU:HD11	1.99	0.45
1:A:375:ARG:O	1:A:379:ASP:HB2	2.16	0.45
1:A:328:PRO:HB3	1:A:418:HIS:CD2	2.51	0.45
1:A:100:SER:C	1:A:101:ASP:O	2.53	0.45
1:A:102:PHE:O	1:A:102:PHE:CD1	2.70	0.45
1:B:375:ARG:O	1:B:379:ASP:HB2	2.16	0.45
1:A:385:ILE:HD11	1:A:412:ILE:HD13	1.98	0.45
1:B:190:ASN:O	1:B:192:PRO:CD	2.65	0.44
1:A:194:CYS:HB2	2:A:901:HEM:ND	2.32	0.44
1:A:488:GLU:HB3	1:A:490:TRP:CE2	2.52	0.44
1:A:290:LYS:HG2	1:A:292:ARG:NH1	2.32	0.44
1:A:77:GLN:O	1:A:78:TYR:HB3	2.18	0.44
1:B:258:LEU:HD13	1:B:347:ALA:HB2	1.99	0.44
1:A:371:GLU:O	1:A:375:ARG:HB2	2.17	0.44
1:B:480:SER:HA	1:B:481:PRO:C	2.38	0.44
1:A:195:ILE:HG12	1:A:458:LEU:CD2	2.42	0.44
1:A:102:PHE:O	1:A:103:THR:CG2	2.65	0.44
1:A:290:LYS:CD	1:A:292:ARG:HH22	2.29	0.44
1:B:141:ILE:HD11	1:B:163:VAL:HG11	2.00	0.44
1:B:88:GLU:C	1:B:89:ILE:HD12	2.38	0.44
1:B:453:ALA:O	1:B:476:ASN:HB2	2.17	0.44
1:A:83:ASN:O	1:A:87:GLY:N	2.50	0.44
1:A:206:PHE:CD2	1:A:239:THR:HG22	2.53	0.43
1:B:188:TRP:HB2	2:B:1901:HEM:CBC	2.48	0.43
1:A:167:ILE:HA	1:A:172:THR:O	2.18	0.43
1:B:351:LEU:HB3	1:B:358:PHE:HB2	1.99	0.43
1:A:377:PHE:O	1:A:385:ILE:HG12	2.17	0.43
1:B:466:ILE:O	1:B:466:ILE:HG22	2.18	0.43
1:A:290:LYS:CG	1:A:292:ARG:HH12	2.30	0.43
1:B:342:ALA:HB1	1:B:425:VAL:HG11	2.00	0.43
1:B:292:ARG:HH12	1:B:297:ASP:HB3	1.82	0.43
1:B:195:ILE:CG1	1:B:458:LEU:HD22	2.49	0.43
1:B:177:LEU:HD13	1:B:177:LEU:C	2.39	0.43
1:A:194:CYS:SG	1:A:197:ARG:HG3	2.58	0.43
1:B:348:ASN:H	1:B:348:ASN:HD22	1.67	0.43
1:A:188:TRP:CD2	1:A:200:TRP:HA	2.53	0.43
1:A:221:ILE:HD12	1:A:303:LEU:HD21	2.01	0.43
1:A:301:LEU:HD12	1:A:301:LEU:HA	1.79	0.43
1:A:266:MET:SD	1:A:272:ARG:HD3	2.58	0.43
1:A:80:ARG:NH2	1:A:89:ILE:HD13	2.34	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:LEU:HD23	1:A:350:LEU:C	2.39	0.43
1:B:262:ALA:HB2	1:B:299:LEU:CD2	2.49	0.43
1:A:234:ILE:HG21	1:A:366:TRP:HB3	2.01	0.42
1:B:134:LEU:HB3	1:B:135:PRO:HD3	2.00	0.42
1:B:136:HIS:O	1:B:139:GLU:HB3	2.19	0.42
1:A:242:PRO:HG2	1:A:251:PHE:CZ	2.54	0.42
1:A:134:LEU:HB3	1:A:135:PRO:HD3	2.02	0.42
2:A:901:HEM:CMC	2:A:901:HEM:HBC2	2.49	0.42
1:A:80:ARG:HH22	1:A:89:ILE:HD13	1.84	0.42
1:A:482:PHE:HB3	1:A:484:TYR:CE1	2.54	0.42
1:A:466:ILE:HG22	1:A:466:ILE:O	2.20	0.42
1:A:124:ARG:CD	5:A:1020:HOH:O	2.63	0.42
1:B:289:TRP:NE1	1:B:314:GLU:OE1	2.51	0.42
1:B:223:ARG:HD3	5:B:1950:HOH:O	2.19	0.42
1:B:327:HIS:CG	1:B:328:PRO:HD2	2.55	0.42
1:A:374:VAL:O	1:A:378:CYS:HB2	2.20	0.42
1:A:195:ILE:HG21	1:A:195:ILE:HD13	1.81	0.42
1:A:327:HIS:CG	1:A:328:PRO:HD2	2.55	0.42
1:A:153:ILE:H	1:A:153:ILE:CD1	2.06	0.41
1:B:188:TRP:CD2	1:B:200:TRP:HA	2.55	0.41
1:A:453:ALA:O	1:A:476:ASN:HB2	2.20	0.41
1:B:257:GLN:CB	1:B:345:ALA:O	2.68	0.41
1:B:182:PHE:CZ	1:B:186:MET:HE2	2.53	0.41
1:B:175:LEU:HD13	1:B:356:LEU:HD11	2.02	0.41
1:B:79:VAL:HG23	1:B:95:HIS:NE2	2.34	0.41
1:B:472:GLN:O	1:B:474:MET:HG2	2.20	0.41
1:A:121:ARG:HD3	1:A:121:ARG:HA	1.87	0.41
1:B:175:LEU:HD13	1:B:356:LEU:HD12	2.03	0.41
1:B:345:ALA:HB2	1:B:364:ASN:HB3	2.03	0.41
1:B:486:GLN:HB2	5:B:1917:HOH:O	2.20	0.41
1:A:444:GLU:OE1	1:A:444:GLU:HA	2.20	0.41
1:A:303:LEU:N	1:A:303:LEU:CD1	2.83	0.41
1:B:283:LEU:O	1:B:287:LEU:HG	2.20	0.41
1:B:305:ALA:O	1:B:307:GLY:N	2.53	0.41
1:A:183:ALA:HB2	1:A:353:VAL:HG21	2.03	0.41
1:A:407:ARG:HD2	5:A:1117:HOH:O	2.21	0.41
1:A:262:ALA:HB2	1:A:299:LEU:HG	2.03	0.41
1:B:163:VAL:O	1:B:167:ILE:HG13	2.21	0.41
1:B:333:PHE:O	1:B:336:LEU:HD23	2.21	0.41
1:A:489:PRO:C	1:A:491:LYS:H	2.25	0.41
1:B:386:LEU:HB2	5:B:1990:HOH:O	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:332:TRP:CE3	1:B:392:ARG:HD2	2.56	0.40
1:B:266:MET:CE	1:B:272:ARG:HE	2.34	0.40
1:B:257:GLN:HB3	1:B:257:GLN:HE21	1.68	0.40
1:A:438:MET:HE3	1:A:469:VAL:HA	2.03	0.40
1:B:161:GLU:CG	1:B:165:LYS:HE2	2.51	0.40
1:A:488:GLU:O	1:A:491:LYS:HB2	2.22	0.40
1:A:254:TRP:HB2	1:A:302:VAL:HB	2.04	0.40
1:B:172:THR:OG1	1:B:173:TYR:N	2.54	0.40

All (8) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:406:ASP:OD2	1:B:463:SER:OG[9_766]	1.72	0.48
1:A:103:THR:CG2	1:A:118:SER:OG[11_655]	1.87	0.33
1:B:231:ASN:N	1:B:318:ASP:OD2[11_656]	1.99	0.21
1:B:318:ASP:N	5:B:1954:HOH:O[11_656]	1.99	0.21
1:A:470:PHE:O	3:A:902:H4B:O9[11_655]	2.00	0.20
1:A:461:PRO:O	1:A:464:GLY:N[11_655]	2.12	0.08
1:B:99:THR:OG1	1:B:478:VAL:O[9_766]	2.12	0.08
1:A:318:ASP:OD2	5:A:1065:HOH:O[9_765]	2.19	0.01

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	411/433 (95%)	370 (90%)	35 (8%)	6 (2%)	13 26
1	B	406/433 (94%)	367 (90%)	38 (9%)	1 (0%)	52 77
All	All	817/866 (94%)	737 (90%)	73 (9%)	7 (1%)	21 42

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	102	PHE
1	A	200	TRP
1	A	306	ASP
1	B	306	ASP
1	A	307	GLY
1	A	369	GLY
1	A	344	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	363/381 (95%)	339 (93%)	24 (7%)	21 40
1	B	358/381 (94%)	328 (92%)	30 (8%)	14 26
All	All	721/762 (95%)	667 (92%)	54 (8%)	17 33

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	94	LEU
1	A	101	ASP
1	A	102	PHE
1	A	114	MET
1	A	125	ASP
1	A	148	PHE
1	A	157	LEU
1	A	161	GLU
1	A	180	LEU
1	A	255	ASN
1	A	257	GLN
1	A	258	LEU
1	A	290	LYS
1	A	301	LEU
1	A	303	LEU
1	A	324	THR
1	A	325	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	338	LEU
1	A	348	ASN
1	A	386	LEU
1	A	395	LEU
1	A	417	LEU
1	A	467	THR
1	A	475	LEU
1	B	78	TYR
1	B	114	MET
1	B	119	LEU
1	B	125	ASP
1	B	128	THR
1	B	130	LEU
1	B	131	GLU
1	B	134	LEU
1	B	148	PHE
1	B	175	LEU
1	B	178	ASP
1	B	186	MET
1	B	210	ASN
1	B	215	GLN
1	B	226	LEU
1	B	233	ASN
1	B	257	GLN
1	B	258	LEU
1	B	292	ARG
1	B	301	LEU
1	B	325	MET
1	B	331	GLU
1	B	348	ASN
1	B	386	LEU
1	B	407	ARG
1	B	417	LEU
1	B	421	GLN
1	B	423	GLN
1	B	462	VAL
1	B	467	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	96	HIS
1	A	142	ASN
1	A	202	ASN
1	A	204	GLN
1	A	215	GLN
1	A	219	GLN
1	A	231	ASN
1	A	233	ASN
1	A	249	HIS
1	A	348	ASN
1	A	471	HIS
1	B	96	HIS
1	B	210	ASN
1	B	231	ASN
1	B	233	ASN
1	B	348	ASN
1	B	423	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	HEM	A	901	-	30,50,50	2.60	10 (33%)	24,82,82	2.34	9 (37%)
3	H4B	A	902	-	13,18,18	1.68	2 (15%)	11,26,26	1.94	5 (45%)
4	A55	A	903	-	21,25,25	1.92	5 (23%)	21,35,35	1.88	4 (19%)
2	HEM	B	1901	-	30,50,50	2.85	12 (40%)	24,82,82	2.14	8 (33%)
3	H4B	B	1902	-	13,18,18	1.76	2 (15%)	11,26,26	1.92	4 (36%)
4	A55	B	904	-	21,25,25	1.88	4 (19%)	21,35,35	1.89	6 (28%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	A	901	-	-	0/10/54/54	0/0/8/8
3	H4B	A	902	-	1/1/3/5	0/8/17/17	0/2/2/2
4	A55	A	903	-	-	0/9/22/22	0/1/3/3
2	HEM	B	1901	-	-	0/10/54/54	0/0/8/8
3	H4B	B	1902	-	-	0/8/17/17	0/2/2/2
4	A55	B	904	-	-	0/9/22/22	0/1/3/3

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1901	HEM	C2D-C3D	-7.21	1.32	1.54
2	A	901	HEM	C2D-C3D	-6.99	1.33	1.54
2	B	1901	HEM	C3B-CAB	-6.27	1.39	1.51
2	B	1901	HEM	C3C-CAC	-6.04	1.40	1.51
2	B	1901	HEM	C3B-C4B	-5.85	1.46	1.51
3	B	1902	H4B	C7-N8	-5.81	1.38	1.46
2	A	901	HEM	C3C-CAC	-5.72	1.40	1.51
3	A	902	H4B	C7-N8	-5.42	1.39	1.46
2	A	901	HEM	C2C-C1C	-4.76	1.43	1.52
2	A	901	HEM	C3D-C4D	-4.69	1.45	1.51
2	A	901	HEM	C3B-CAB	-4.65	1.42	1.51
2	B	1901	HEM	C3D-C4D	-2.73	1.48	1.51
2	B	1901	HEM	C2C-C1C	-2.68	1.47	1.52
2	A	901	HEM	CAD-C3D	-2.67	1.48	1.54
2	A	901	HEM	C2B-C1B	-2.37	1.44	1.51
2	B	1901	HEM	C2B-C1B	-2.28	1.44	1.51
3	A	902	H4B	C4A-N5	-2.16	1.33	1.38
3	B	1902	H4B	C4A-N5	-2.05	1.33	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	904	A55	C1-C2	2.02	1.42	1.38
4	B	904	A55	O22-C20	2.04	1.27	1.23
2	B	1901	HEM	C4C-NC	2.10	1.38	1.36
2	A	901	HEM	C4C-NC	2.21	1.38	1.36
4	A	903	A55	C1-C6	2.23	1.42	1.38
2	B	1901	HEM	FE-NB	2.25	2.09	1.97
2	B	1901	HEM	CHC-C1C	2.31	1.41	1.36
4	A	903	A55	O22-C20	2.31	1.28	1.23
2	A	901	HEM	C1C-NC	2.49	1.39	1.36
4	A	903	A55	C1-C2	2.52	1.43	1.38
2	B	1901	HEM	FE-NC	2.85	2.07	1.95
2	A	901	HEM	FE-NC	2.89	2.07	1.95
4	A	903	A55	C10-N9	3.60	1.33	1.28
2	B	1901	HEM	C1C-NC	3.87	1.40	1.36
4	B	904	A55	C10-N9	4.20	1.33	1.28
4	B	904	A55	C5-C10	5.01	1.53	1.46
4	A	903	A55	C5-C10	5.17	1.53	1.46

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	901	HEM	CBA-CAA-C2A	-3.21	106.77	112.53
4	A	903	A55	C5-C10-N11	-2.70	117.35	120.13
4	B	904	A55	C5-C10-N11	-2.63	117.42	120.13
4	A	903	A55	C2-C3-C4	-2.52	119.70	122.81
4	B	904	A55	C16-C8-N7	-2.51	105.80	110.94
3	A	902	H4B	N3-C2-N1	-2.23	121.87	125.53
4	B	904	A55	C2-C3-C4	-2.20	120.10	122.81
3	B	1902	H4B	N3-C2-N1	-2.18	121.96	125.53
4	A	903	A55	C1-C6-C5	-2.17	119.66	123.42
2	A	901	HEM	C3B-C4B-CHC	2.04	126.04	123.16
4	B	904	A55	N11-C10-N9	2.08	121.87	118.77
2	B	1901	HEM	C3B-CAB-CBB	2.08	127.65	124.46
2	A	901	HEM	CAA-C2A-C1A	2.16	129.35	127.01
3	A	902	H4B	C2-N1-C8A	2.19	119.47	114.54
2	B	1901	HEM	C3B-C4B-CHC	2.34	126.46	123.16
2	B	1901	HEM	CMD-C2D-C3D	2.48	125.31	114.35
3	B	1902	H4B	C2-N1-C8A	2.48	120.12	114.54
3	A	902	H4B	C7-C6-N5	2.51	115.66	110.45
3	B	1902	H4B	C4-C4A-C8A	2.82	117.12	114.56
4	B	904	A55	C16-C8-N9	2.89	113.88	109.48
3	A	902	H4B	C4-C4A-C8A	2.92	117.20	114.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1901	HEM	CAD-C3D-C2D	2.96	121.73	113.22
3	A	902	H4B	C4-N3-C2	2.99	120.09	115.94
3	B	1902	H4B	C4-N3-C2	3.11	120.25	115.94
2	B	1901	HEM	CMB-C2B-C3B	3.29	124.74	116.53
2	A	901	HEM	CMB-C2B-C3B	3.30	124.76	116.53
2	A	901	HEM	CAD-C3D-C2D	3.52	123.33	113.22
2	A	901	HEM	C3B-CAB-CBB	3.63	130.02	124.46
2	A	901	HEM	CAD-C3D-C4D	3.98	126.52	112.47
2	B	1901	HEM	CMC-C2C-C3C	4.37	127.43	116.53
2	B	1901	HEM	C2D-C3D-C4D	4.51	109.14	101.50
2	B	1901	HEM	CAD-C3D-C4D	4.55	128.53	112.47
2	A	901	HEM	C2D-C3D-C4D	4.93	109.86	101.50
4	B	904	A55	C5-C4-C3	4.94	121.57	117.72
2	A	901	HEM	CMC-C2C-C3C	4.96	128.90	116.53
4	A	903	A55	C5-C4-C3	5.26	121.82	117.72

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	902	H4B	C6

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	HEM	3	0
3	A	902	H4B	0	1
2	B	1901	HEM	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	415/433 (95%)	1.52	102 (24%)	1	0	26, 45, 74, 99	0
1	B	410/433 (94%)	1.61	121 (29%)	1	0	25, 43, 68, 94	0
All	All	825/866 (95%)	1.56	223 (27%)	1	0	25, 44, 70, 99	0

All (223) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	108	SER	7.8
1	B	494	ILE	7.5
1	A	102	PHE	7.3
1	B	87	GLY	6.6
1	B	110	LEU	6.4
1	A	171	GLY	6.1
1	A	101	ASP	5.9
1	A	103	THR	5.6
1	B	109	CYS	5.3
1	A	211	CYS	5.2
1	B	170	THR	5.0
1	B	400	LEU	5.0
1	A	494	ILE	4.5
1	A	232	GLY	4.5
1	A	390	GLY	4.2
1	A	283	LEU	4.1
1	B	277	THR	4.1
1	A	275	ALA	4.0
1	B	298	VAL	3.9
1	A	118	SER	3.9
1	B	89	ILE	3.9
1	B	290	LYS	3.8
1	B	200	TRP	3.8
1	A	89	ILE	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	237	ALA	3.7
1	B	340	TRP	3.7
1	A	291	PRO	3.6
1	A	409	VAL	3.6
1	B	267	PRO	3.5
1	B	330	TYR	3.5
1	A	161	GLU	3.5
1	B	416	VAL	3.5
1	B	489	PRO	3.4
1	B	84	TRP	3.4
1	A	164	THR	3.4
1	B	451	CYS	3.4
1	B	495	TRP	3.4
1	B	397	THR	3.4
1	B	117	LYS	3.4
1	B	192	PRO	3.4
1	B	420	PHE	3.4
1	A	110	LEU	3.4
1	A	150	GLU	3.4
1	A	276	ALA	3.4
1	A	152	LYS	3.3
1	B	144	TYR	3.3
1	A	423	GLN	3.3
1	B	269	GLY	3.3
1	A	136	HIS	3.3
1	A	263	GLY	3.2
1	B	372	ILE	3.2
1	B	169	THR	3.2
1	A	321	LEU	3.2
1	B	123	PRO	3.2
1	B	194	CYS	3.1
1	A	415	ALA	3.1
1	B	350	LEU	3.1
1	A	292	ARG	3.1
1	B	95	HIS	3.1
1	A	236	SER	3.1
1	A	212	SER	3.0
1	B	152	LYS	3.0
1	B	148	PHE	3.0
1	B	446	ARG	3.0
1	A	441	MET	2.9
1	B	303	LEU	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	125	ASP	2.9
1	B	251	PHE	2.9
1	B	475	LEU	2.9
1	B	447	ALA	2.9
1	A	141	ILE	2.9
1	B	196	GLY	2.9
1	A	79	VAL	2.9
1	A	495	TRP	2.9
1	B	249	HIS	2.9
1	B	80	ARG	2.9
1	B	440	HIS	2.8
1	B	191	ALA	2.8
1	B	483	TYR	2.8
1	B	261	TYR	2.8
1	B	145	TYR	2.8
1	B	125	ASP	2.8
1	B	288	GLY	2.8
1	B	430	HIS	2.7
1	B	392	ARG	2.7
1	A	241	PHE	2.7
1	B	338	LEU	2.7
1	A	412	ILE	2.7
1	B	305	ALA	2.7
1	B	155	GLU	2.7
1	B	90	LEU	2.7
1	B	454	ASP	2.7
1	B	342	ALA	2.7
1	B	481	PRO	2.7
1	A	391	ARG	2.7
1	B	138	ILE	2.7
1	B	412	ILE	2.7
1	B	272	ARG	2.6
1	A	367	TYR	2.6
1	A	452	PRO	2.6
1	A	122	GLY	2.6
1	A	149	LYS	2.6
1	B	437	PHE	2.6
1	A	229	THR	2.6
1	B	239	THR	2.6
1	B	395	LEU	2.6
1	B	163	VAL	2.6
1	B	206	PHE	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	283	LEU	2.5
1	A	124	ARG	2.5
1	A	361	CYS	2.5
1	B	188	TRP	2.5
1	A	366	TRP	2.5
1	A	306	ASP	2.5
1	B	294	GLY	2.5
1	B	262	ALA	2.5
1	B	439	LYS	2.5
1	A	179	GLU	2.5
1	B	445	TYR	2.5
1	A	203	LEU	2.4
1	A	259	ILE	2.4
1	B	314	GLU	2.4
1	A	323	VAL	2.4
1	B	425	VAL	2.4
1	B	337	GLY	2.4
1	A	308	GLN	2.4
1	B	334	GLN	2.4
1	B	436	SER	2.4
1	A	476	ASN	2.4
1	A	78	TYR	2.4
1	B	85	GLY	2.4
1	B	453	ALA	2.4
1	A	471	HIS	2.4
1	A	389	VAL	2.3
1	B	379	ASP	2.3
1	B	432	THR	2.3
1	A	442	GLN	2.3
1	A	80	ARG	2.3
1	A	416	VAL	2.3
1	B	366	TRP	2.3
1	B	306	ASP	2.3
1	A	251	PHE	2.3
1	A	336	LEU	2.3
1	A	329	LYS	2.3
1	A	231	ASN	2.3
1	A	312	VAL	2.3
1	A	396	GLU	2.3
1	A	382	ARG	2.3
1	B	190	ASN	2.3
1	A	195	ILE	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	225	ILE	2.3
1	A	445	TYR	2.3
1	A	111	GLY	2.3
1	B	426	THR	2.3
1	A	262	ALA	2.3
1	A	302	VAL	2.3
1	A	414	VAL	2.3
1	A	153	ILE	2.3
1	A	123	PRO	2.2
1	A	360	ALA	2.2
1	B	93	THR	2.2
1	A	77	GLN	2.2
1	A	128	THR	2.2
1	A	278	LEU	2.2
1	A	148	PHE	2.2
1	A	337	GLY	2.2
1	A	385	ILE	2.2
1	A	492	THR	2.2
1	A	485	TYR	2.2
1	B	160	LEU	2.2
1	B	343	LEU	2.2
1	B	448	ARG	2.2
1	B	409	VAL	2.2
1	A	303	LEU	2.2
1	A	420	PHE	2.2
1	B	273	GLY	2.2
1	B	353	VAL	2.2
1	A	189	ARG	2.2
1	B	278	LEU	2.1
1	B	142	ASN	2.1
1	B	171	GLY	2.1
1	A	483	TYR	2.1
1	B	433	ALA	2.1
1	B	375	ARG	2.1
1	A	387	GLU	2.1
1	A	112	SER	2.1
1	B	402	SER	2.1
1	B	195	ILE	2.1
1	B	291	PRO	2.1
1	B	136	HIS	2.1
1	A	90	LEU	2.1
1	A	310	PRO	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	460	PRO	2.1
1	B	96	HIS	2.1
1	A	488	GLU	2.1
1	A	254	TRP	2.1
1	B	271	ILE	2.1
1	B	241	PHE	2.1
1	B	362	PRO	2.1
1	B	78	TYR	2.1
1	A	209	ARG	2.1
1	A	295	ARG	2.1
1	A	344	PRO	2.1
1	A	446	ARG	2.1
1	A	475	LEU	2.1
1	B	226	LEU	2.1
1	A	120	THR	2.1
1	B	394	GLY	2.1
1	B	275	ALA	2.1
1	B	114	MET	2.0
1	B	354	GLY	2.0
1	B	458	LEU	2.0
1	B	205	VAL	2.0
1	B	459	VAL	2.0
1	B	150	GLU	2.0
1	B	181	ILE	2.0
1	B	474	MET	2.0
1	A	477	TYR	2.0
1	B	231	ASN	2.0
1	B	326	GLU	2.0
1	B	381	GLN	2.0
1	B	210	ASN	2.0
1	B	382	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	A55	B	904	23/23	0.64	0.46	3.44	23,31,54,56	0
2	HEM	B	1901	43/43	0.74	0.35	1.22	23,25,29,37	0
3	H4B	B	1902	17/17	0.68	0.34	0.81	26,29,34,34	0
4	A55	A	903	23/23	0.69	0.32	0.52	28,32,46,48	0
2	HEM	A	901	43/43	0.81	0.27	-0.77	24,26,30,30	0
3	H4B	A	902	17/17	0.84	0.21	-2.69	28,30,31,32	0

6.5 Other polymers (i)

There are no such residues in this entry.